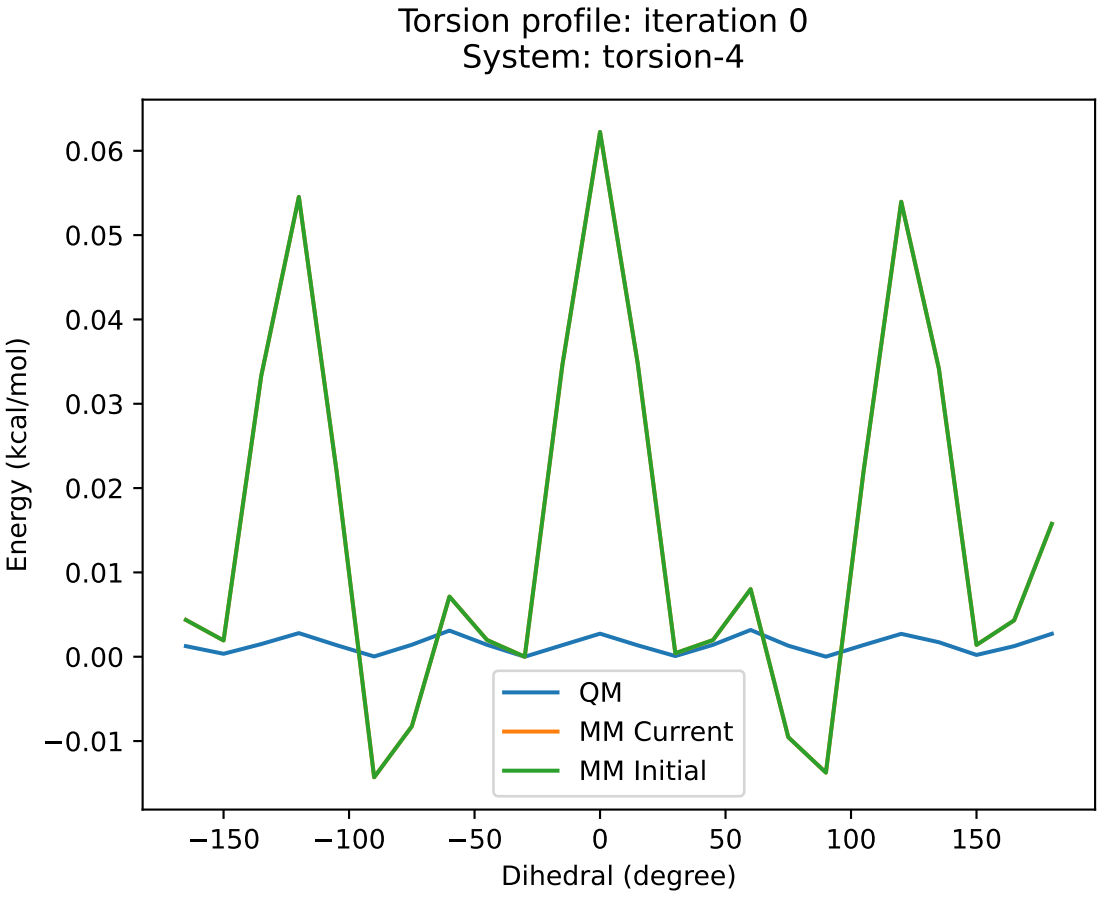
Torsion profile: iteration 0
System: torsion-4
Energy (kcal/mol)
0.06
0.05
0.04
0.03
0.02
0.01
0.00
−0.01
−150
−100
−50
0
50
100
150
Dihedral (degree)
QM
MM Current
MM Initial